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(FILE 'HOME' ENTERED AT 11:04:01 ON 08 JUL 2004)

FILE 'REGISTRY' ENTERED AT 11:05:19 ON 08 JUL 2004
L1 1 S NICARDIPINE/CN
L2 1 S NIFEDIPINE/CN

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L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 21829-25-4 REGISTRY
CN 3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(2-nitrophenyl)-, dimethyl ester (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(o-nitrophenyl)-, dimethyl ester (8CI)
OTHER NAMES:
CN 2,6-Dimethyl-3,5-dicarbomethoxy-4-(2-nitrophenyl)-1,4-dihydropyridine
CN 2,6-Dimethyl-4-(2-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylic acid dimethyl ester
CN 4-(2-Nitrophenyl)-2,6-dimethyl-3,5-dicarbomethoxy-1,4-dihydropyridine
CN Adalat
CN Adalat 10
CN Adalat 20
CN Adalat 5
CN Adalat CC
CN Adalat CR
CN Adalat Crono
CN Adalat FT
CN Adalat GITS
CN Adalat GITS 30
CN Adalat LA
CN Adalat LP
CN Adalat Oros
CN Adalat PA
CN Adalat Retard
CN Adalate
CN Adapine
CN Adapress
CN Alat
CN Aldipin
CN Alfadat
CN Alonix
CN Alonix S
CN Alpha-Nifedipine Retard
CN Angipec
CN Anifed
CN Anpine
CN Apo-Nifed
CN Aprical
CN BAY 1040
CN BAY-a 1040
CN Bonacid
CN Calcibloc
CN Calcigard
CN Calcilat
CN Camont
CN Cardifen
CN Cardilat
CN Cardilate
CN Cardionorm
CN Chronadalate
CN Chronadalate LP
CN Citilat
CN Coracten
CN Coral
CN Cordafen

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H donors (HD)	1		(1) ACD
Koc (KOC)	2.13	pH 1	(1) ACD
Koc (KOC)	587	pH 4	(1) ACD
Koc (KOC)	1090	pH 7	(1) ACD
Koc (KOC)	1091	pH 8	(1) ACD
Koc (KOC)	1091	pH 10	(1) ACD
logD (LOGD)	0.34	pH 1	(1) ACD
logD (LOGD)	2.78	pH 4	(1) ACD
logD (LOGD)	3.05	pH 7	(1) ACD
logD (LOGD)	3.05	pH 8	(1) ACD
logD (LOGD)	3.05	pH 10	(1) ACD
logP (LOGP)	3.054+/-0.590		(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	346.33		(1) ACD
pKa (PKA)	3.93+/-0.20	Most Basic	(1) ACD
Vapor Pressure (VP)	3.37E-09 Torr	25 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.67 ((C) 1994-2004 ACD/Labs)

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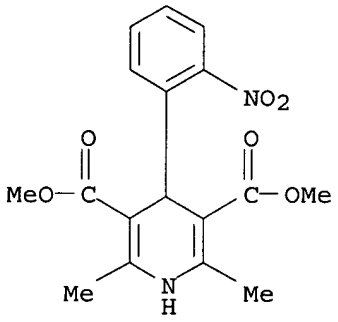
CN **Nifedipine**
ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT - Use FCN, FIDE, or ALL for DISPLAY
FS 3D CONCORD
DR 11104-22-6, 101539-70-2, 101554-38-5
MF C17 H18 N2 O6
CI COM
LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DIOGENES, DRUGU, EMBASE, IFICDB, IFIPAT, IFIUDB, IMSCOSEARCH, IMSPATENTS, IPA, MEDLINE, MRCK*, MSDS-OHS, NIOSHTIC, PHAR, PROMT, PROUSDDR, PS, RTECS*, SPECINFO, TOXCENTER, USAN, USPAT2, USPATFULL, VETU
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, WHO
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Book; Conference; Dissertation; Journal; Patent; Report
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
RLD.P Roles for non-specific derivatives from patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7031 REFERENCES IN FILE CA (1907 TO DATE)
102 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
7047 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d scan l2

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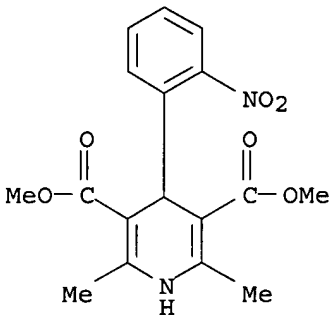
IN 3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(2-nitrophenyl)-, dimethyl ester (9CI)
ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT
MF C17 H18 N2 O6
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> d prop l2

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN

Experimental Properties (EPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Melting Point (MP)	172-174 deg C		(1) IC
Melting Point (MP)	172-173 deg C	Solv: methanol (67-56-1)	(2) IC

(1) Cupka, Pavol; CS 243590 B1 1987 CAPLUS
(2) Loev, Bernard; Journal of Medicinal Chemistry 1974 V17(9) P956-65 CAPLUS

Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1	pH 1	(1) ACD
Bioconc. Factor (BCF)	66.3	pH 4	(1) ACD
Bioconc. Factor (BCF)	123	pH 7	(1) ACD
Bioconc. Factor (BCF)	123	pH 8	(1) ACD
Bioconc. Factor (BCF)	123	pH 10	(1) ACD
Boiling Point (BP)	475.3+/-45.0 deg C	760 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	73.87+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	241.2+/-51.7 deg C		(1) ACD
H acceptors (HAC)	8		(1) ACD

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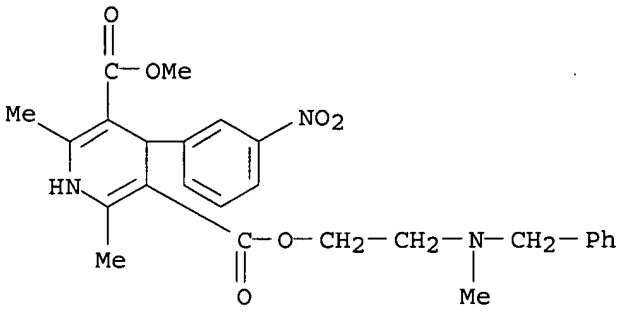
L1 1 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, methyl 2-[methyl(phenylmethyl)amino]ethyl ester (9CI)
MF C26 H29 N3 O6
CI COM



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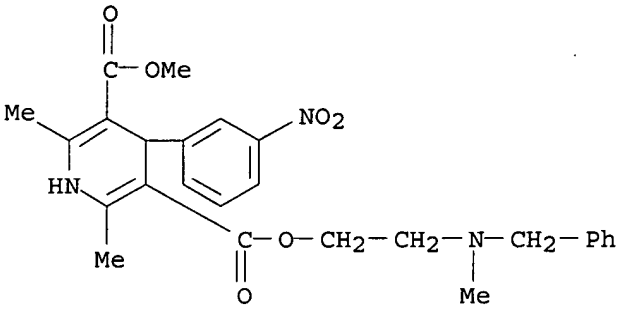
L1 1 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, methyl 2-[methyl(phenylmethyl)amino]ethyl ester (9CI)
MF C26 H29 N3 O6
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> d prop

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN

Experimental Properties (EPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Melting Point (MP)	168.5 deg C	Solv: acetone (67-64-1)	(1) IC

(1) Nakamoto, Yasumasa; JP 62059261 A2 1987 CAPLUS

Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1	pH 1	(1) ACD
Bioconc. Factor (BCF)	5.04	pH 4	(1) ACD
Bioconc. Factor (BCF)	2395	pH 7	(1) ACD
Bioconc. Factor (BCF)	4841	pH 8	(1) ACD
Bioconc. Factor (BCF)	5454	pH 10	(1) ACD
Boiling Point (BP)	603.4+/-55.0 deg C	760 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	89.75+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	318.7+/-56.7 deg C		(1) ACD
H acceptors (HAC)	9		(1) ACD
H donors (HD)	1		(1) ACD
Koc (KOC)	1	pH 1	(1) ACD

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Koc (KOC)	15.2	pH 4	(1) ACD
Koc (KOC)	7220	pH 7	(1) ACD
Koc (KOC)	14592	pH 8	(1) ACD
Koc (KOC)	16440	pH 10	(1) ACD
logD (LOGD)	0.27	pH 1	(1) ACD
logD (LOGD)	2.19	pH 4	(1) ACD
logD (LOGD)	4.86	pH 7	(1) ACD
logD (LOGD)	5.17	pH 8	(1) ACD
logD (LOGD)	5.22	pH 10	(1) ACD
logP (LOGP)	5.221+/-0.622		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	479.53		(1) ACD
pKa (PKA)	7.11+/-0.20	Most Basic	(1) ACD
Vapor Pressure (VP)	1.63E-14 Torr	25 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.67 ((C) 1994-2004 ACD/Labs)

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